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Ladder operators for the Coulomb potential

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Abstract : The ladder operators for the non-relativistic quantum Coulomb problem are obtained by solving a linear system of first-order differential equations. This approach being simpler than standard ones.

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The Schrödinger equation for a hydrogen-like atom with nuclear charge Ze is [1] ($h = m = 1$) :

$$-\frac{1}{2}\left[\frac{d^2}{dr^2}-\frac{l(l+1)}{r^2}\right]\psi_{nl}(r)-\frac{Ze^2}{r}\psi_{nl}(r)$$
$$\frac{Z^2e^4}{2n^2}\psi_{nl}(r), \qquad (1)$$

where Z is the atomic number, e the electron charge, $\frac{1}{r}\psi_{nl}$ is the hydrogenic radial wave function, $n = 1, 2, 3, \ldots$ is the principal quantum number, and $l = 0, 1, \ldots, n-1$ is the orbital quantum number.

This paper has the goal of determining ladder operators $A^{\pm}_{nl}$ for a given value of n, such that

$$\psi_{n,l\pm1}(r) = A^{\pm}_{nl}\psi_{nl}(r). \qquad (2)$$

In this way, given the state ψ_{n0} we can obtain all the states ψ_{nl} applying the operator A^{+}_{nl} an approppriate number of times; for example, $\psi_{n1} = A^{+}_{n0}\psi_{n0}$ and so on. Otherwise, we might use A^{-}_{nl} to get all the ψ_{nl} starting with $\psi_{n,n-1}$.

There are various methods proposed for getting this kind of ladder operators; for example, the procedure used in [2] requires the explicit expression of ψ_{nl}, but this is not necessary in the technique proposed in this work. It neither needs to invoke the factorization method [3–9] to deduce $A^{\pm}_{nl}$ as is done by certain authors [3,10]. There are various other methods [11] where the ladder operators are obtained taking advantage of the mapping [12–16] relating the Coulomb with the Morse [7,17–22] problem. In this work we take a different approach and propose that the ladder operators may be written as

$$A^{+}_{nl} = f(r)\frac{d^2}{dr^2}+g(r)\frac{d}{dr}+h(r) \qquad (3)$$

and show that eq. (1) and (2) lead to a system of linear first-order differential equations for f, g and h. As a matter of fact, we explicitly do the calculations only for A^{+}_{nl} since those for A^{-}_{nl} follow a similar process.

If we define the operator

$$B_{nl} = -\frac{1}{2}\left[\frac{d^2}{dr^2}-\frac{l(l+1)}{r^2}\right]-\frac{Ze^2}{r}\cdot\frac{Z^2e^4}{2n^2} \qquad (4)$$

then eq. (1) can be rewritten as

$$B_{nl}\psi_{nl} = 0. \qquad (5)$$

Use of eq. (5) for $\psi_{n,l+1}$ together with the relevant component of eq. (2) allows as to obtain $B_{n,l+1}A^{+}_{nl}\psi_{nl} = 0$, that is

$$\left\{\left[B_{n,l+1}, A^{+}_{nl}\right]+A^{+}_{nl}B_{n,l+1}\right\}\psi_{nl} = 0, \qquad (6)$$

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where $[C,D]$ stands for the commutator of C and D. From eq. (4) it follows that $B_{n,l+1} = B_{nl} + (l+1)/r^2$, which may be substituted into (6) and together with eq. (5) it leads to

$$\vartheta_{nl}\psi_{nl} = 0,$$

with $$\vartheta_{nl} = \left[B_{n,l+1}, A_{nl}^{+}\right] + (l+1)A_{nl}^{+}\frac{1}{r^2}\cdot \tag{7}$$

Eq. (7) is satisfied if we impose the condition $\vartheta_{nl} = 0$, which in union with relations (3) and (5) leads to the following set of equations

$$f' = 0; \tag{8}$$

$$g' + \frac{1}{2}f'' - (l+1)\frac{f}{r^2} = 0, \tag{9}$$

$$h' + \frac{2}{r^2}\left[Ze^2 + \frac{l(l+1)}{r}\right]f + \frac{1}{2}g'' - (l+1)\frac{g}{r^2} = 0, \tag{10}$$

$$\frac{1}{2}h'' - (l+1)\frac{h}{r^2} - \frac{Ze^2}{r^2}\left(\frac{2f}{r} - g\right) + \frac{l(l+1)}{r^3}\left(\frac{3f}{r} - g\right) = 0, \tag{11}$$

where the primes represent r-derivatives. Eq. (8) imply that $f(r) = C_1$, a constant, which together with (9) implies a first order differential equation for $g(r)$ whose solution is $g(r) = C_2 - (l+1)C_1/r$. The last function $h(r)$ in cq. (3) can now be obtained by solving (10) :

$$h(r) = C_3 + \frac{1}{r}\left[2Ze^2C_1 - C_2(l+1)\right] + \frac{3C_1}{2}\, l(l+1).$$

Finally, the expressions for f, g and h are substituted into equation (11) to get $C_1 = 0$ and $C_2 = (l+1)C_3/Ze^2$, from which we deduce

$$A_{nl}^{+} = \frac{(l+1)}{Ze^2}C_3\left(\frac{d}{dr} + \frac{Ze^2}{l+1} - \frac{l+1}{r}\right). \tag{12}$$

The constant $C_3 \equiv G_{nl}$ is determined using recurrence; in fact, from (2) and (12) we have that $\psi_{n1} = A_{n0}^{+}\psi_{n0} = G_{n0} \times$ function (r) but the normalization condition $\int_0^\infty \psi_{n1}^2 dr = 1$ implies $G_{n0}^2 = n^2/(n^2-1)$. Similarly $\psi_{n2} = A_{n1}^{+}\psi_{n1} = G_{n1}G_{n0} \times$ function (r) together with $\int_0^\infty \psi_{n2}^2 dr = 1$ implies $G_{n1}^2 = n^2/(n^2-4)$, and so on. It is not difficult to obtain an expression for C_3, which is $C_3 = -n\left[n^2 - (l+1)^2\right]^{-1/2}$. In this way, equation (12) becomes equivalent to eq. (42) in ref. [11].

In an analogous fashion we can show that the lowering operator

$$A_{nl}^{-} = \frac{nl}{Ze^2\sqrt{n^2 - l^2}}\left(\frac{d}{dr} - \frac{Ze^2}{l} + \frac{l}{r}\right) \tag{13}$$

satisfies eq. (2).

We have shown that determining the ladder operators $A_{nl}^{\pm}$ is equivalent to solving a set of linear first-order differential equations. The operators (12) and (13) are equivalent to those obtained by others [10,23] using the factorization method or supersymmetric techniques and, as it is known, they are very useful for evaluating matrix elements of radial functions [24,25].

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